Eigensolvers and Applications in Finite Element Analyses

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SUMMARY

This article presents an overview of eigenproblems that arise in current finite-element computations. We focus on a set of applications that have been studied at CERFACS, Centre Européen de Recherche et de Formation Avancée en Calcul Scientifique, and describe the ideas and tools that have been developed to deal with them. The main characteristics of five different cases are given. We also discuss the trends as well as the research efforts to understand and tackle new applications.

1 INTRODUCTION

The solution of the equation

$$Ax = \lambda Bx \tag{1}$$

where A and B are $n \times n$ matrices, x is a non null vector and λ is a scalar, has long been an important computation. We recall here that relation (1) defines a *generalized eigenproblem*; a *standard eigenproblem* is obtained when B is equal to the identity matrix I. Usually, the n possible pairs (λ, x), *eigenvalues* λ and *eigenvectors* x, that satisfy relation (1) are associated with fundamental characteristics of differential and integral operators describing a physical phenomenon. In some applications from chemistry, for instance, they are related to basic configurations of molecules (hinge-bending motions); in nuclear power plants, neutron fluxes (the behaviour is super-critical for a dominant eigenvalue greater than one); and in structural engineering, dynamic properties of a given model (natural vibration frequencies and mode shapes). Depending on the complexity, the level of the discretization of a continuous problem or the precision required for the results, A and B can reach dimensions of tens of thousands. In practical analyses only a few *eigenpairs* (λ, x) are considered relevant, either in the extremities of the spectrum (lower or upper), in an interval (ξ_1, ξ_2) for real solutions or in a region for complex ones. Although only few are wanted, their evaluation is usually a time consuming task. The characteristics of a given problem, such as the sparsity of the operators, should be thus taken into account. Whether only the eigenvalues or eigenvectors are required becomes also an important issue. Therefore, the development of new eigensolvers, or the improvement of existing ones, has been the subject of continuous research [8,18,21,22,25].

Krylov subspace based methods such as Lanczos [19] and Arnoldi [21] algorithms have been widely used for treating eigenproblems associated with very large sparse matrices. They can be shown to perform better than vector iteration (inverse or direct), transformation methods (Jacobi, Householder or Givens) or determinant search in many practical cases. See [7] and [19] for an overview of those techniques. The Krylov subspace associated with a matrix A and a non null starting vector q_1 is defined as

$$\mathcal{K}(A, q_1, j) = span(q_1, Aq_1, ...A^{j-1}q_1). \tag{2}$$

The goal of the Lanczos algorithm is the generation of a basis for the Krylov subspace, so that the orthogonal projection of the original problem into the basis leads to a smaller problem, involving a tridiagonal matrix (which is symmetric if A is). Eigensolutions of A are then recovered through a Rayleigh-Ritz procedure [19]. Conversely, the projection computed by Arnoldi's method involves a Hessenberg matrix (if A is nonsymmetric) [21]. Within block Krylov strategies, the starting vector q_1 is replaced by a full rank $n \times p$ matrix Q_1, $1 < p \ll n$, which allows for better convergence properties when there are multiple eigenvalues and can provide better data management on some computer architectures. Block tridiagonal and block Hessenberg matrices are then obtained as projections. The solution of the reduced problem is in general easy to perform. Moreover, the good news is that, with Lanczos and Arnoldi based procedures, approximate solutions $(\hat{\lambda}, \hat{x})$ are usually obtained even for small values of j for the associated Krylov subspace (2) [7,19]. An estimation of the residual $\|A\hat{x} - \hat{\lambda}B\hat{x}\|_2$ ($\|.\|_2$ is the 2-norm) can be obtained at very low cost during the basis generation process, so that $\hat{x}$ is computed only when it is accurate enough.

The objective of this work is to give an overview of eigenproblems that arise in current finite element computations and techniques to deal with them. We have opted not to give further details about computational performance, the modelling of the physical phenomena or the finite-element formulations. We focus on the applications being examined at CERFACS, *Centre Européen de Recherche et de Formation Avancée en Calcul Scientifique*, for which both eigenvalues and eigenvectors are required. In the next section, we briefly describe the ideas and tools developed at CERFACS for the solution of very large sparse eigenproblems. In the following, we list a set of applications and their main characteristics. The first application is a classic from structural engineering: the determination of free vibration solutions in dynamic analyses, the challenge now being the really huge problems. The others are rather innovative: real unsymmetric problems in flutter analysis, spectral portrait computations, a particular case of the Maxwell equations, and quadratic eigenproblems associated with electromagnetic waveguides. Finally, we discuss the trends in the field as well as the present research efforts to understand and tackle new applications.

2 KRYLOV SUBSPACE BASED METHODS

Let us consider the standard eigenproblem and assume that the basis for the Krylov subspace generated by A is given by $\mathbf{Q}_j = [q_1, q_2, ... q_j]$, $\mathbf{Q}_j^T \mathbf{Q}_j = I$, computed by either the Lanczos or Arnoldi method. The solutions of the projected (reduced) problem are assumed to be (θ_i, s_i), $i = 1, 2, ...j$. Then, approximate pairs $(\hat{\lambda}, \hat{x})$ are obtained by means of [7,19]

$$\hat{x} = \mathbf{Q}_j s_i,$$
$$\hat{\lambda} = \theta_i.$$

When the problem is generalized, it can be rewritten as $\hat{A}y = \lambda y$, where $\hat{A} = (L^{-1} A L^{-T})$ and $x = L^{-T} y$, providing B can be factorized as LL^T. Another possibility is $\hat{A}x = (\frac{1}{\lambda})x$ with $\hat{A} = (A^{-1}B)$, providing A is invertible (actually A does not need to be explicitly inverted, a solution of a system of equations may be performed instead for the basis generation). In such cases, the basis of vectors are built with the operator $\hat{A}$. If both A and B are singular, a translation of origin may be applied on their characteristic polynomials. See [10, ch. 10 by Nour-Omid, B.] and [19, ch. 15] for more details. We assume that $B = I$ for simplicity and first describe the Lanczos and Arnoldi methods regardless of roundoff errors. Then, we make some general remarks upon both techniques and the tools developed at CERFACS.

2.1 The Lanczos Algorithm: Hermitian Matrices

For a Hermitian matrix A, $q_0 = 0$, and a starting vector q_1, $q_1^T q_1 = 1$, the Lanczos basis generation process can be expressed by the recurrence

$$q_{j+1}\beta_{j+1} = r_j = Aq_j - q_j\alpha_j - q_{j-1}\beta_j \tag{3}$$

where α_j and β_j are scalars for the Gram-Schmidt orthogonalization of q_j and q_{j-1} with respect to Aq_j, and $\beta_{j+1} = \|r_j\|_2$. Then, $Ax = \lambda x$ is projected into $T_j s = \theta s$ (i.e., $\mathbf{Q}_j^T A \mathbf{Q}_j = T_j$), where T_j is a symmetric tridiagonal matrix: $t_{i,j} = 0$ whenever $|i - j| > 1$, $t_{j,j} = \alpha_j$ and $t_{j,j+1} = t_{j+1,j} = \beta_{j+1}$.

2.2 The Arnoldi Algorithm: Non Hermitian Matrices

For a non Hermitian matrix A and a starting vector q_1, $q_1^T q_1 = 1$, the Arnoldi basis generation process can be expressed by the recurrence

$$q_{j+1}h_{j+1,j} = r_j = Aq_j - \sum_{i=1}^{j} q_i h_{i,j} \tag{4}$$

where $h_{i,j}$ are scalars for the Gram-Schmidt orthogonalization of q_i, $i = 1, 2, ...j$, with respect to Aq_j, and $h_{j+1,j} = \|r_j\|_2$. Then, $Ax = \lambda x$ is projected into $H_j s = \theta s$ (i.e., $\mathbf{Q}_j^T A \mathbf{Q}_j = H_j$), where H_j is a Hessenberg matrix with coefficients $h_{i,j}$, which are 0 for $i \geq j + 2$.

2.3 Lanczos and Arnoldi: general remarks

If the techniques are implemented as just described, a loss of orthogonality among the vectors in $\mathbf{Q}_j$ is generally observed after some steps. It is the result of roundoff errors in recurrences (3)-(4), and the convergence of pairs $(\hat{\lambda}, \hat{x})$ as well [7,19]. Once orthogonality is lost, redundant copies of eigenpairs tend to appear. Therefore, preventive measures, such as selective orthogonalization or partial reorthogonalization, are commonly employed to control and keep the orthogonality of $\mathbf{Q}_j$ within a certain level. See [8], [10, ch. 10 by Nour-Omid, B.] and [19] for more information.

It is usually assumed (and observed) that the Lanczos and Arnoldi algorithms find solutions at the extremities of the spectrum. Their convergence pattern, however, is strongly related to the eigenvalue distribution. Therefore, for the determination of interior solutions or those of small real part, a preconditioning (shift-invert, polynomials) is generally required [21]. The maximum allowable j can also be reached without the convergence of all desired solutions. Then, restarting is an alternative way to proceed and different strategies exist for that purpose [21,22].

2.4 Packages developed at CERFACS

Two main packages which are described below have been developed at CERFACS for the solution of very large eigenproblems:

a) `BLZPACK` is an implementation of the block Lanczos algorithm for the solution of real symmetric eigenproblems [13]. It is intended for the solution of $Ax = \lambda Bx$ with A positive definite and B semi positive definite or equal to I. Solutions in a specific interval (ξ_1, ξ_2) or close to a value σ can be found by an automatic transformation of the original problem into $B(A-\sigma B)^{-1}Bx = (\frac{1}{\lambda-\sigma})Bx$. The matrices A and B are not required internally in the code, so that each time a computation involving either A or B has to be performed, the control is returned to the user (and such a computation can be specialized for particular applications).

b) `ARNCHEB` is an implementation of the Arnoldi-Tchebycheff algorithm for the solution of eigenproblems involving non Hermitian matrices [2,3,4]. The package can be applied to problems $Ax = \lambda Bx$ where A is real and $B = I$ (a collaboration between CERFACS and Aerospatiale), A complex and $B = I$, and A complex and B Hermitian positive definite or complex. CG and GMRES type iterative methods or the LU factorization may be used for finding solutions in specific regions of the complex plane. In addition, the implementation is particularly robust to highly nonnormal operators. A nonnormal operator A satisfies $\|A^TA - AA^T\|_2 \neq 0$, which can lead to numerical difficulties for many applications.

Portability and performance for the aforementioned packages are achieved by using BLAS kernels and other public domain tools (EISPACK and LAPACK). The accuracy of the computed solutions is carefully evaluated by a norm of the type $\|\hat{A}\hat{x} - \hat{\lambda}\hat{x}\|_2 / \|\hat{A}\|_2 \leq tol$. Moreover, efficient techniques are used to ensure an adequate level of orthogonality among the vectors of the basis $\mathbf{Q}_j$, overcoming problems caused by finite precision arithmetic.

3 APPLICATIONS

In this section, we describe five different applications related to finite elements computations. We focus on the eigenproblems obtained instead of the associated physical phenomena and the element formulation. The objective is to give an idea of the kind of emerging problems that arise when promising techniques and high performance computers are at hand. The cases presented form a rather small but illustrative set. All of them have been studied with Krylov based techniques such as those available in `BLZPACK` and `ARNCHEB`. For quadratic eigenproblems, however, some tools are still being developed.

3.1 Structural Analysis

The evaluation of dynamic responses in structural engineering analysis often requires the solution of the equation

$$M\ddot{u} + C\dot{u} + Ku = f(t) \tag{5}$$

where M, C and K are the sparse symmetric mass, damping and stiffness matrices of the model, $\ddot{u}$, $\dot{u}$ and u are the accelerations, velocities and displacements, and $f(t)$ are the time dependent forces. Depending on the formulation used for C, the responses for that equation can be obtained by means of the solutions of the associated eigenproblem [1,10]

$$K\phi = \omega^2 M\phi \tag{6}$$

where ω is a *free vibration frequency* and ϕ a *mode shape*. Furthermore, the frequencies and modes allow good insight into the structural model [1,14,23]. The dimensions of M and K reach many thousands for current applications (such as engine and automobile finite element discretizations) and dimensions as high as 10^6 have already been reported.

The free vibration problem defined in (6) can be efficiently solved in any interval of interest if a shift-invert approach is feasible. With such a strategy, we deal with the transformed problem [8,17]

$$M(K - \sigma M)^{-1} M\phi = (\frac{1}{\lambda - \sigma})M\phi.$$

No inversion needs to be performed in practice, since one can generate a Lanczos basis solving systems of equations through the factorization $(K - \sigma M) = LDL^T$ for a well chosen σ (based on the interval of interest). It is well known, however, that such a factorization may be computationally expensive for large problems. In addition, the matrix $(K - \sigma M)$ may be indefinite so that care has to taken during the factorization process [7]. Nevertheless, with that approach the determination and validation of the sought solutions is feasible, which is an important and attractive feature. `BLZPACK`, referred to in the previous section, allows the use of different factorization and storage schemes in a convenient way. Efficient and reliable implementations of factorization strategies are available in [9], for instance, using sparse storage schemes. If the matrices are stored in skyline form, which is common practice in 2-dimensional finite element analyses, a partitioned LDL^T can be employed. The idea is to work with pieces of the matrix (copied to and from temporary arrays), as shown in Figure 1, together with matrix-vector products to perform the required calculations. This combination leads to very good performance on computers with hierarchical memories [11], in spite of some overhead introduced by handling the skyline storage.

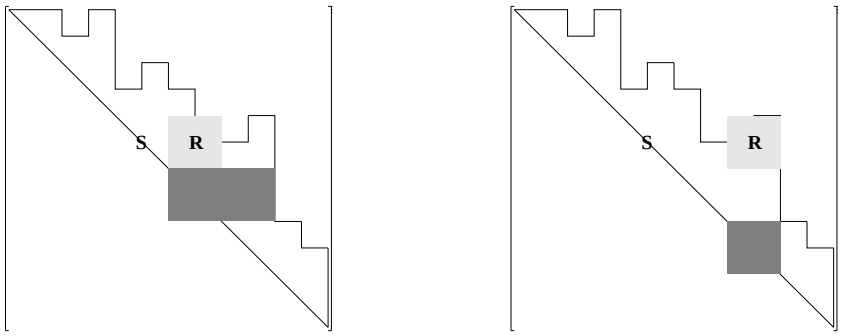


Figure 1. Partitioned factorization.

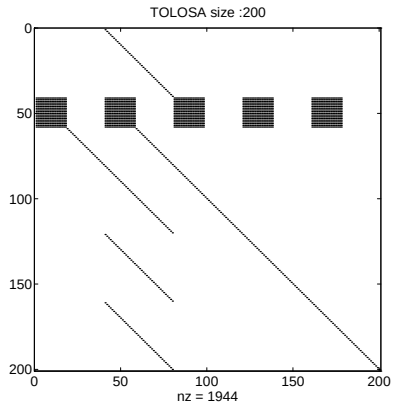
3.2 Unsymmetric Problems

Unsymmetric problems appear now in many different fields, such as fluid dynamics. However, we show here a problem proposed by the Structural Research and Development Department at Aerospatiale, in Toulouse. It corresponds to the modelling of a *flutter* phenomenon, with a coupling of a torsional vibration and a bending motion of a wing in flight [2,3,4,5]. In such a case, the equation of motion (5) is "corrected" to

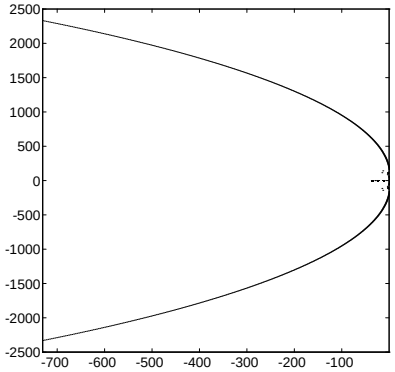
$$M\ddot{u} + Ku = F\dot{u} \tag{7}$$

where F is nonsymmetric and nonnormal, corresponding to an estimation of the aerodynamic contribution of the discretization points. Then, equation (7)

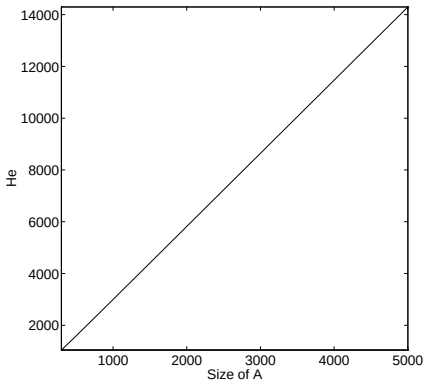
can be solved through the eigenpairs of a problem $Ax = \lambda x$, where A is highly nonnormal, possibly leading to numerical difficulties [2,3,4]. Actually, a whole family of matrices, labeled *Tolosa* [6], has been obtained for the application described, depending on the discretization employed. For large values of n the matrices have multiple and possibly defective eigenvalues. From the aeroelasticity point of view the eigenvalues of interest are those of largest imaginary part. The Figure 2 shows some characteristics of *Tolosa*: a) the pattern of a matrix of dimension 200, b) the eigenvalues of a matrix of dimension 2000, c) the departure from normality, $He = \|A^TA - AA^T\|_2/\|A^2\|_2$, as a function of the dimension, and d) the norm, $\|A\|_2$, as a function of the dimension. One can observe, for instance, that the norm of A varies exponentially with its dimension while the departure from normality varies linearly. The information provided by *Tolosa* was valuable to the understanding of nonnormality effects and to develop robust eigenvalue codes such as `ARNCHEB`.



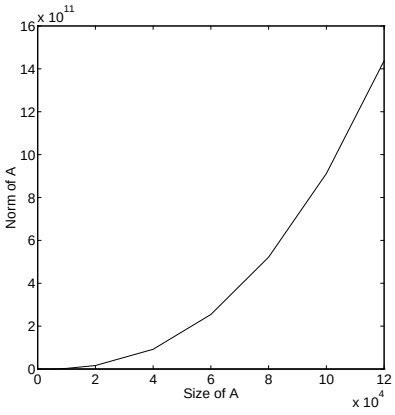
a) Pattern of Tolosa, $n = 200$.



b) Spectrum of Tolosa, $n = 2000$.



c) Tolosa, departure from normality.



d) Tolosa, $\|A\|$.

Figure 2. Tolosa, a flutter analysis.

3.3 Spectral Portrait Computations

Many computations involving nonsymmetric matrices may fail in the neighbourhood of singularities. This is basically related to finite precision arithmetic and the nonnormality of the operators. While a matrix A has eigenvalues λ, a matrix $A + \Delta A$ has eigenvalues $\lambda + \Delta\lambda$, where ΔA indicates an arbitrary perturbation. However, due to the physical and numerical properties of a particular problem, $\Delta\lambda$ can be large even for a small ΔA. Situations like this happen in fluid dynamics and electromagnetism applications [4].

One way of studying the "sensitivity" of a matrix consists in the introduction of small perturbations to the entries of the matrix and then examining its resulting perturbed spectrum [15,16]. The perturbed spectrum can be analyzed through the function

$$\psi(z) = \log_{10}[\|(A - zI)^{-1}\|_2 \|A\|_2],$$

where z corresponds to a point in the complex plane and $\|(A - zI)^{-1}\|_2$ to the largest singular value of $(A - zI)^{-1}$. However, it should be noted that this singular value is equivalent to

$$1/\sqrt{\lambda_{min}[(A - zI)^*(A - zI)]}$$

where λ_{min} indicates the smallest eigenvalue and the * the conjugate transpose [15,16]. We describe here the utilization of a Hermitian-Lanczos code [12] to determine the spectral portrait $\psi(z)$ of a nonsymmetric matrix, i.e., to compute the largest singular value for different values of z. The idea consists in running the code with the Hermitian matrix $(A - zI)^*(A - zI)$ until the smallest eigenvalue of the reduced problem reaches a small residual, which is examined outside the code (reverse communication strategy). Alternatively, the code can be applied to the augmented Hermitian matrix

$$\begin{bmatrix} 0 & A \\ A^* & 0 \end{bmatrix}$$

which has better numerical properties [16]. The matrix studied has dimension 135 and comes from the *Tolosa* family described in the previous section. The spectral portrait obtained is shown in Figure 3, for 16641 values of z (mesh 128×128), in the region of the complex plane defined by the points $(-300 - 250i)$, $(-300 + 250i)$, $(200 - 250i)$ and $(200 + 250i)$. In that figure, the vertical and horizontal axes give the complex and real parts of the plane, respectively, and the light colours indicate large values of $\psi(z)$. In other words, those colours indicate the perturbations for which the spectrum of A suffers important modifications, or the set of eigenvalues of any $A + \Delta A$, where $\|\Delta A\|_2 \leq \epsilon \|A\|_2$, $\epsilon = 10^{-16}$ being the machine (double) precision. The spectral portrait then gives an idea of the values that could be erroneously considered as eigenvalues.

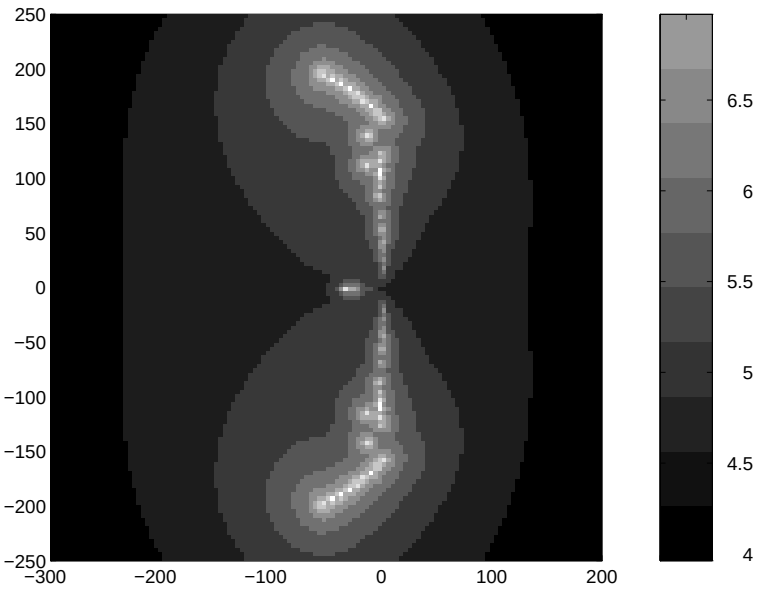


Figure 3. The spectral portrait of Tolosa.

3.4 Complex Non Hermitian Problems

In the study of electromagnetic guided waves, the electric and magnetic fields, respectively E and H, considering a heterogeneous media and the harmonic case, are given by the Maxwell equations [4]

$$\begin{aligned} rot_\beta E + i\omega H &= 0, \\ rot_\beta H - i\omega E &= 0, \\ div_\beta(\rho E) &= 0, \\ div_\beta(\mu H) &= 0, \end{aligned}$$

where i is the complex unit, ω the wave frequency, β a propagation constant, μ the magnetic permeability and ρ the dielectric permittivity of the media. Those equations can be discretized by means of a Lagrangian finite-element formulation. The admissible values of ω are then obtained as a function of β, by solving a standard eigenvalue problem involving a complex non-Hermitian matrix based on E or alternatively on H. A generalized eigenvalue problem involving complex non-Hermitian matrices in also a variant. We consider a system of the former type, with dimension 105. Its eigenvalue spectrum is shown in Figure 4 and its singular values are represented in Figure 5. The package `ARNCHEB` has been applied to study the eigenvalue distribution of this problem using complex versions of CG and GMRES type methods [2,3]. The singular value distribution has been studied with the same Hermitian-Lanczos code mentioned in the previous section and an augmented matrix formulation [12]. The singular value decomposition is a clever way of determining the matrix rank and therefore is a useful tool in the analysis of systems of equations, for instance [7].

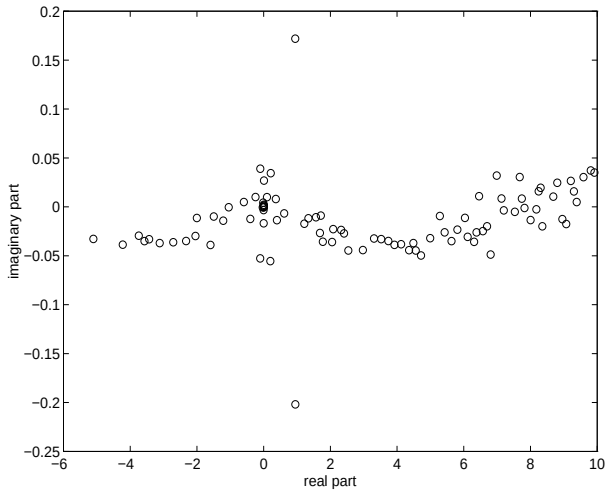


Figure 4. Guided waves, spectrum of a sample matrix.

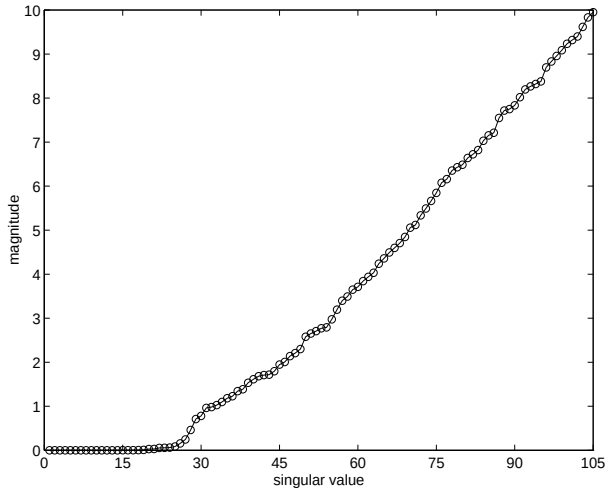


Figure 5. Guided waves, singular values of a sample matrix.

3.5 Quadratic Problems

Quadratic eigenproblems result, for instance, from the solution of equation (5) for particular C's, the solution of the Navier-Stokes equation or the study of propagation modes in optical fibers. Such problems usually admit complex solutions and can be linearized through an augmented system approach. Different strategies can be then applied to solve the linearized problem, yielding a symmetric generalized eigensystem with indefinite matrices or a nonsymmetric standard one.

We consider here an application in optical fibers [24]. For a given frequency ω, the goal is to find solutions (modes) of Maxwell equations for sinusoidal fields of the form

$$\mathbf{E}(x,y,z) = \mathbf{e}(x,y)e^{-i\beta z} = (\mathbf{e}_t(x,y) + \boldsymbol{e}_z(x,y)\mathbf{a}_z)e^{-i\beta z}$$

which represents an electric field propagation in the z-direction. The complex scalar β is a *mode propagation constant* and the vector $\mathbf{e}$ is projected along the waveguide axis $\boldsymbol{e}_z$ and on the transverse plane $\mathbf{e}_t$. Using vector infinite elements the problem above is rewritten as

$$\begin{aligned} \beta^2 B x_1 + \beta C^T x_2 - A x_1 &= 0 \\ \beta C x_1 + D x_2 &= 0 \end{aligned}$$

where x_1 and x_2 are approximate solutions and A, B, C and D are built with the basis functions of the approximated subspace. A and B are $n \times n$, D is $m \times m$, C is $m \times n$, and $n \approx 3 \times m$. All matrices are real and sparse, A and D are indefinite and B is positive definite. With a transformation of the type $u = \beta x_1$, $v = x_2$ we can define

$$\begin{bmatrix} A & 0 \\ 0 & 0 \end{bmatrix} \begin{Bmatrix} u \\ v \end{Bmatrix} = \lambda \begin{bmatrix} B & C^T \\ C & D \end{bmatrix} \begin{Bmatrix} u \\ v \end{Bmatrix} \tag{7}$$

or $\boldsymbol{A}x = \lambda \boldsymbol{B}x$, where $\lambda = \beta^2$. The matrices $\boldsymbol{A}$ and $\boldsymbol{B}$ are indefinite so that complex solutions may exist. In addition, spurious zeros solutions are artificially introduced in (7) due to the structure of $\boldsymbol{A}$. The patterns of $\boldsymbol{A}$ and $\boldsymbol{B}$ may look like those depicted in Figure 6, for $n = 190$ and $m = 63$. The corresponding eigenvalue distribution (λ) is given in Figure 7.

A Lanczos based code is being developed to study this problem, following the ideas proposed by Parlett and Chen in [20]. The purpose is to project $\boldsymbol{A}x = \lambda \boldsymbol{B}x$ into $T_j s = \theta \Omega_j s$, so that the basis of vectors satisfies $\mathbf{Q}_j^T \boldsymbol{B} \mathbf{Q}_j = \Omega_j$, with the matrices T_j and Ω_j reflecting the indefiniteness of the original ones. An important issue here is that one can obtain a breakdown of the type $q_j^T \boldsymbol{B} q_j = 0$ for $q_j \neq 0$. A "look-ahead" scheme is then important for assuring a reliable implementation.

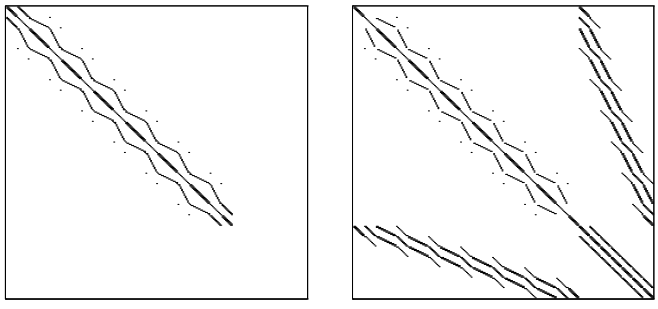


Figure 6. Typical patterns of $\boldsymbol{A}$ and $\boldsymbol{B}$.

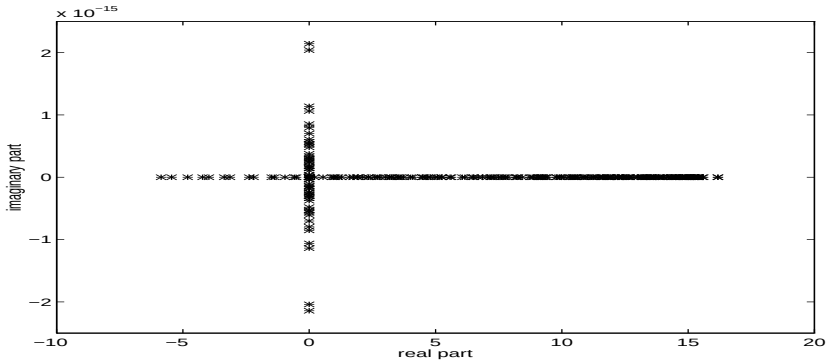


Figure 7. Eigenvalue distribution of $\boldsymbol{A}x = \lambda \boldsymbol{B}x$.

4 CONCLUSIONS

The solution of eigenvalue problems is of extreme importance to understand many physical phenomena. Therefore, this work listed a non exhaustive set of eigenvalue applications arising in different fields, where finite element procedures allow for their modelling and solution. Eigenvalue calculations, however, use to be costly computational tasks because as the techniques and computers evolve so do the complexity and size of the applications. It is a consensus that the computer architectures together with new applications will influence the eigensolutions extraction softwares. In many cases, factorizations for a shift-invert approach are not feasible anymore. In molecular self-consistent-field computations using a p-version finite element (3-D), for instance, the objective is to reach discretizations leading to up to 300^3 or 1000^3 unknowns. Hundreds of eigenpairs would be then desirable for the solution of the associated Hartree-Fock or Schroedinger equations. However, the current packages (if any computer memory) seem not to be suited for that. The use and development of new tools (as preconditionings) are very important to deal with such huge problems.

Currently, there is a proposal for a TMR (Training and Mobility of Researchers) project to study, develop and analyze important problems in both academic and industrial worlds at an European level. The partners are University of Athens, University of Manchester, University of Umeå, CERFACS, Rutherford Appleton Laboratory, Aerospatiale and Thomson-CSF. The project has been labeled RELEASE, for Reliable and Efficient Solution of Large-Scale Eigenproblems. There is also an ALLIANCE proposal submitted by the University of Wales at Swansea and CERFACS to study algorithms for the free vibration analysis and optimization of complex vibrating shell structures, which are efficient when implemented on high performance computers. These examples of collaboration illustrate the effort to tackle and understand new problems, keeping a good pace to attend on the future demands.

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Additional documentation

Additional documentation on the mentioned problems as well as some test problems themselves is available by anonymous ftp at ftp.cerfacs.fr (138.63.200.222), directory /pub/algo/reports, or at the URL http://www.cerfacs.fr/algor/algoreports.html.

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